

**TOUGH**  
symposium  
2003



# **TOUGH Symposium 2003**

**Lawrence Berkeley National Laboratory**

**Berkeley, California**

**May 12–14, 2003**

**Technical Program**

# **TOUGH Symposium 2003**

**Lawrence Berkeley National Laboratory**

**Berkeley, California**

**May 12–14, 2003**

## **Technical Program**

### **Monday Morning, May 12, 2003, Building 66 Auditorium**

07:30 – 08:30 Registration

08:30 – 08:45 Karsten Pruess

08:45 – 09:00 Organizing Committee

Welcome

Introduction and Announcements

## Monday Morning, May 12, 2003, Building 66 Auditorium

### Session 1: Geothermal Reservoir Engineering

Chairman: Marcelo Lippmann, Lawrence Berkeley National Laboratory, Berkeley, California

- 09:00 – 09:30 *Grimur Björnsson, Arnar Hjartarson, Gudmundur Bodvarsson, Benedikt Steingrímsson* *Development of a 3-D geothermal reservoir model for the greater Hengill volcano in SW-Iceland*
- 09:30 – 09:50 Cornel Ofwona *An update of the natural state numerical model of Olkaria geothermal system, Kenya*
- 09:50 – 10:10 Claudio Calore, Alfredo Battistelli *Application of TOUGH2/EWASG to the modelling of salt water injection into a depleted geothermal reservoir: preliminary results*
- 10:10 – 10:40 *Coffee Break*
- 10:40 – 11:00 Kazumi Osato, Satoshi Ujo, Stephen White *Prediction of formation equilibrium temperature while drilling based on drilling mud temperature: Inverse problem using TOUGH2 and wellbore thermal model*
- 11:00 – 11:20 Micol Todesco, Jonny Rutqvist, Giovanni Chiodini, Karsten Pruess, Curt Oldenburg *Modeling of recent volcanic episodes at Phlegrean Fields (Italy): Geochemical variations and ground deformation*
- 11:20 – 11:40 Pat Dobson, Sonia Salah, Nicolas Spycher, Eric Sonnenthal *Simulation of water-rock interaction in the Yellowstone geothermal system using TOUGHREACT*
- 11:40 – 13:00 *Lunch Break, LBNL Cafeteria*

## Monday Afternoon, May 12, 2003, Building 66 Auditorium

### Session 2: Fracture Flow and Vadose Zone Hydrology

Chairman: Paul Witherspoon, University of California, Berkeley, California

13:00 – 13:30	<i>Stefan Finsterle</i>	<i>iTOUGH2: From parameter estimation to model structure identification</i>
13:30 – 13:50	Robert Podgorney, Jerry Fairley	Evaluating conceptual models of flow in unsaturated, fractured porous media
13:50 – 14:10	Hui-Hai Liu, Guoxiang Zhang, Gudmundur Bodvarsson	The Active Fracture Model: Its relation to fractal flow patterns and further evaluation using field observations
14:10 – 14:30	Ivan Lunati, Wolfgang Kinzelbach	Gas tracer tests in an unsaturated fracture: Water soluble gases as partitioning tracers
14:30 – 15:00		<i>Coffee Break</i>
15:00 – 15:20	Niclas Bockgård, Auli Niemi	Role of soil-rock interaction on recharge into fractured rock
15:20 – 15:40	Alan Flint	The role of unsaturated flow in artificial recharge projects
15:40 – 16:00	Michael Kowalsky, Stefan Finsterle, Yoram Rubin	Estimating flow parameters using ground-penetrating radar and hydrological data during transient flow in the vadose zone

## **Monday Evening, May 12, 2003, Cafeteria**

### **Session 3: Poster Session**

Chairman: Curt Oldenburg, Lawrence Berkeley National Laboratory, Berkeley, California

17:00 – 20:00

*Poster Session*

#### **Session 3.1: New Modules and Developments**

Jong Kim, Stefan Finsterle	Application of automatic differentiation in TOUGH2
Karsten Pruess, Alfredo Battistelli	TMVOC, a simulator for multiple volatile organic chemicals
Chao Shan, Karsten Pruess	EOSN—A new TOUGH2 module for simulating transport of noble gases in the subsurface

#### **Session 3.2: Pre- and Post-Processing**

Daniel Swenson, Brian Hardeman, Casey Presson, Charlie Thornton	Using PetraSim to create, execute, and post-process TOUGH2 models
Kazumasa Ito, Yongkoo Seol	A 3-dimensional discrete fracture network generator to examine fracture-matrix interaction using TOUGH2
Lehua Pan	WinGridder—An interactive grid generator for TOUGH2
John Burnell, Stephen White, Kazumi Osato, Tatsuya Sato	GeoCad—A pre- and postprocessor for TOUGH2
Tatsuya Sato, Kazumi Ohsato, Takahiro Shiga	G-Star-Base (G*Base)—A data base system for underground information and post-processing for TOUGH2

### **Session 3.3: Geothermal Engineering**

Jason McKenna, David Blackwell

Numerical modeling of transient basin and range extensional geothermal systems

Tatsuya Sato, Kazumi Ohsato,  
Takahiro Shiga, Masatake Sato,  
Stephen White, Warwick Kissling

A study of reservoir estimation for a deep-seated geothermal reservoir using TOUGH2 and CHEMTOUGH2

Alexey Kiryukhin, V. Yampolski

Modeling study of the Pauzhetsky geothermal field, Kamchatka, Russia

Yvette Ontoy, Phil Molling,  
Nicolas Spycher, Tianfu Xu,  
Mauro Parini, Karsten Pruess

Scaling of hot brine injection wells: Supplementing field studies with reactive transport modeling

### **Session 3.4: Gas Transport and Vadose Zone Hydrology**

Alfredo Battistelli, Curt Oldenburg,  
George Moridis, Karsten Pruess

Modeling gas reservoir processes with TMVOC V.2.0

Julio García, Karsten Pruess

Flow instabilities during injection of CO<sub>2</sub> into saline aquifers

Curt Oldenburg, André Unger

Coupled subsurface-surface layer gas transport and dispersion for geologic carbon sequestration seepage simulation

Wenbin Wang, Shlomo Neuman,  
Tzung-mow Yao, Peter Wierenga

Comparative simulations of a large-scale field infiltration experiment

### **Session 3.5: Nuclear Waste Isolation**

Rick Ahlers, Teamrat Ghezzehei, Stefan Finsterle	Development and testing of a method for efficient simulation of evaporation from a seepage face
Irina Engelhardt	Inverse modeling of gas, water, and heat flow in bentonite/crushed rock backfill
Teamrat Ghezzehei, Stefan Finsterle, Robert Trautz	Evaluating the effectiveness of liquid diversion around an underground opening when evaporation is non-negligible
George Moridis, Yongkoo Seol, Yu-Shu Wu	Modeling studies of mountain-scale radionuclide transport in the unsaturated zone at Yucca Mountain, Nevada
André Unger, Stefan Finsterle, Gudmundur Bodvarsson	Estimating large-scale fractured rock properties from radon data collected in a ventilated tunnel

### **Session 3.6: Environmental Engineering**

Alex Lee	3-D numerical modeling of freshwater lens on atoll islands
Quanlin Zhou, Jens Birkholzer, Iraj Javandel, Preston Jordan	Simulation of groundwater flow at the LBNL using TOUGH2
Jeongkon Kim, Franklin Schwartz, Jianyou Shi, Tianfu Xu	Modeling the coupling between flow and transport developed by chemical reactions and density differences using TOUGHREACT

## Tuesday Morning, May 13, 2003, Building 66 Auditorium

### Session 4: Nuclear Waste

Chairman: Alan Flint, U.S. Geological Survey, Sacramento, California

09:00 – 09:30	<i>Gudmundur Bodvarsson,</i> Jens Birkholzer, Stefan Finsterle, Hui-Hai Liu, Jonny Rutqvist, Yu-Shu Wu	<i>The use of TOUGH2/iTOUGH2 in support of the Yucca Mountain Project: Successes and limitations</i>
09:30 – 09:50	Rainer Senger, Bill Lanyon, Paul Marschall, Stratis Vomvoris, Kenichi Ando	TOUGH2/iTOUGH2 modeling in support of the gas migration test (GMT) at the Grimsel Test Site (Switzerland)
09:50 – 10:10	Keni Zhang, Yu-Shu Wu, Chris Ding, Karsten Pruess	TOUGH2_MP: A parallel version of TOUGH2
10:10 – 10:30	Joachim Poppei, Gerhard Mayer, Jean Croisé	Modelling of resaturation, gas migration and thermal effects in a SF/ILW repository in low-permeability over-consolidated clay-shale
10:30 – 11:00		<i>Coffee Break</i>
11:00 – 11:20	Vijen Javeri	Analysis of nuclide transport including non-linear adsorption depending on variable salinity in the heterogeneous geosphere of the Gorleben channel
11:20 – 11:40	Yu-Shu Wu, Guoping Lu Keni Zhang, Bo Bodvarsson	A mountain-scale model for characterizing unsaturated flow and transport in fractured tuffs of Yucca Mountain
11:40 – 12:00	Jens Birkholzer, Sumit Mukhopadhyay, Yvonne Tsang	Modeling water seepage into heated waste emplacement drifts at Yucca Mountain
12:00 – 13:30		<i>Lunch Break, LBNL Cafeteria</i>



## **Tuesday Afternoon, May 13, 2003, Building 66 Auditorium**

### **Session 5: Mining Engineering**

Chairman: Kazumi Osato, Geothermal Energy Research and Development Company (GERD), Tokyo, Japan

13:30 – 14:00	Stephen White, Ashley Creighton, Paul Bixley, Warwick Kissling	<i>Modelling the dewatering and depressurisation of the Lihir open pit gold mine</i>
14:00 – 14:20	Yannick Scheid, Stephan Semprich, A. Chinkulkijniwat	Computation of laboratory test results to estimate the loss of air in compressed air tunnelling
14:20 – 14:40	Jonny Rutqvist, Chin-Fu Tsang	TOUGH-FLAC: a numerical simulator for analysis of coupled thermal-hydrologic-mechanical processes in fractured rock under multi-phase flow condition
14:40 – 15:00		<i>Coffee Break</i>

### **Session 6: Reactive Transport**

Chairman: Jens Birkholzer, Lawrence Berkeley National Laboratory, Berkeley, California

15:00 – 15:30	Alfredo Battistelli	<i>Modeling the biodegradation of organic contaminants with TMVOCbio</i>
15:30 – 15:50	Tianfu Xu, Eric Sonnenthal, Nicolas Spycher, Karsten Pruess	TOUGHREACT: A new code of the TOUGH family of non-isothermal multiphase reactive geochemical transport in variably saturated geologic media
15:50 – 16:10	Michael Singleton, Eric Sonnenthal, Mark Conrad, Don DePaolo	Numerical modeling of stable isotope fractionation and multiphase reactive transport of water vapor using TOUGHREACT
16:10 – 16:30	Stephan Lorenz, Wolfgang Müller	Modelling of halite formation in natural gas storage aquifers
16:30 – 16:50	Eric Sonnenthal, Nicolas Spycher, Tianfu Xu	Linking reaction, transport, and hydrological parameters in unsaturated fractured rock: TOUGHREACT implementation and application
17:30 – 21:00		<i>Conference Dinner, LBNL Cafeteria</i>

## Wednesday Morning, May 14, 2003, Building 50 Auditorium

### Session 7: Environmental Remediation

Chairman: Auli Niemi, Uppsala University, Sweden

08:30 – 09:00	Ron Falta	<i>Simulation of subgridblock scale DNAPL pool dissolution using a dual domain approach</i>
09:00 – 09:20	Terhi Kling, Juhani Korkealaakso	Nonisothermal multiphase modeling as an integration tool in the planning, control and optimization of in situ soil remediation in Söderkulla, southern Finland
09:20 – 09:40	Fritjov Fagerlund, Auli Niemi	Multi-constituent modelling of a gasoline spill using the T2VOC numerical simulator
09:40 – 10:00	Steve Webb, James Phelan	Implementation of land surface boundary conditions in TOUGH2
10:00 – 10:30		<i>Coffee Break</i>

### Session 8: Gas Transport

Chairman: Vijen Javeri, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS), Köln, Germany

10:30 – 11:00	Karsten Pruess	<i>Numerical simulation of leakage from a geologic disposal reservoir for CO<sub>2</sub>, with transitions between super- and sub-critical conditions</i>
11:00 – 11:20	Christine Doughty, Karsten Pruess	Modeling supercritical CO <sub>2</sub> injection in heterogeneous porous media
11:20 – 11:40	Curt Oldenburg	Carbon sequestration in natural gas reservoirs: Enhanced gas recovery and natural gas storage
11:40 – 12:00	George Moridis, Timothy Collett	Strategies for gas production from hydrate accumulations under various geological and reservoir conditions
12:00 – 13:00		<i>Lunch Break, LBNL Cafeteria</i>

## **Wednesday Afternoon, May 14, 2003, Building 50 Auditorium**

### **Session 9: Tricks-of-the-Trade**

Chairman: Stephen P. White, Industrial Research Ltd., Lower Hutt, New Zealand

13:00 – 13:30 Karl Taylor

Evaluation and intercomparison of climate models

13:30 – 14:45 Participants

Two-slide, three-minute presentations: TOUGH problem—SMART solution

Please inform the Organizing Committee about your contribution to this session or submit short description of TOUGH problem.

14:45 – 15:00

*Coffee Break*

### **Session 10: Panel Discussion**

Chairman: Karsten Pruess, Lawrence Berkeley National Laboratory, Berkeley, California

15:00 – 16:00 Ron Falt

Panel discussion

Alan Flint

George Moridis

Steve Webb

Steve White